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Activation of Gold on Titania: Adsorption and Reaction of SO2 on Au/TiO2(110)

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Introduction: Gold particles supported on titania are active catalysts for the low-temperature oxidation of CO, the selective oxidation of propene, and photocatalytic oxidations used for environmental cleanup [1]. Several models have been proposed for explaining the activation of supported gold from special electronic properties resulting from the limited size of the active gold particles (usually less than 10 nm) to the effects of metal-support interactions [2]. In principle, the active sites for the catalytic reactions could be located only on the support Au particles or on the perimeter of the gold-oxide interfaces. Understanding of the interactions of SO_2 with TiO_2(110) single crystals is very important for developing more efficient catalysts or sorbents for pollution control.

Methods and Materials: A single crystal TiO_2(110) was investigated as model systems for SO_2 adsorption using synchrotron-based high-resolution soft X-ray photoemission (SXPS) and first-principles density functional (DF) slab calculations.

Results: The deposition of Au nanoparticles on TiO_2(110) produces a system with an extraordinary ability to adsorb and dissociate SO_2. In this respect, Au/TiO_2 is much more chemically active than metallic gold or stoichiometric titania. On Au(111) and rough polycrystalline surfaces of gold, SO_2 bonds weakly (adsorption energy < 10 kcal/mol) and desorbs intact at temperatures below 200 K. For the adsorption of SO_2 on TiO_2(110) at 300 K, SO_4 is the only products ($SO_2 + O_{oxide} \rightarrow SO_{4,ads}$). In contrast, Au/$TiO_2$(110) surfaces fully dissociates the SO_2 molecules under identical reaction conditions. The Au$\leftrightarrow$$TiO_2$ interactions are complex and simultaneously enhance the $DeSO_x$ activity of both gold and titania. Once Au bonds to titania, its ability to adsorb and dissociate SO_2 largely increases. In addition, Au adatoms modify the rate of exchange of O vacancies between the bulk and surface of titania, enhancing in this way the chemical activity of the oxide. The behavior the SO_2/Au/TiO_2(110) system illustrates the importance of surface and subsurface O vacancies when dealing with the chemical properties of gold/titania.

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